

# MODIFIED GROUP PROJECTORS: TIGHT BINDING METHOD

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**Abstract.** Modified group projector technique for induced representations is a powerful tool for calculation and symmetry quantum numbers assignation of a tight binding Hamiltonian energy bands of crystals. Namely, the induced type structure of such a Hamiltonian enables efficient application of the procedure: only the interior representations of the orbit stabilizers are to be considered. Then the generalized Bloch eigen functions are obtained naturally by the expansion to the whole state space. The method is applied to the electronic  $\pi$ -bands of the single wall nanotubes: together with dispersion relations, their complete symmetry assignation by the full symmetry (line) groups and the corresponding symmetry-adapted eigen function are found.

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## 1. Introduction

Let  $S$  be the system with the symmetry group  $\mathbf{G}$ . The group action divides the system into (disjoint) orbits and the total system state space decomposes onto the orbital subspaces. Each orbital space is induced from the so called interior space of a single atom of that orbit. Accordingly, in the state space  $\mathcal{S} = \mathcal{S}_D$  the group acts by the representation  $D(\mathbf{G})$  decomposing onto the induced type orbital subrepresentations. Typical examples are crystals; consisted of the orbits of the translational group, their symmetry-adapted eigen states are suitable linear combinations of the Bloch states, corresponding to the energy band structure. The symmetry-adapted or standard basis (SAB) can be found by the group projector technique. Here we develop and apply its efficient modification [1] free of the difficulties emerging from the non-compactness of the involved groups.

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Let  $D(\mathbf{G})$  decomposes onto the irreducible components  $D^{(\mu)}(\mathbf{G})$  as  $D(\mathbf{G}) = \oplus_{\mu} a_{\mu} D^{(\mu)}(\mathbf{G})$  ( $a_{\mu} = 1, 2, \dots$ ). The basis  $\{ | \mu t_{\mu} m \rangle | \mu; t_{\mu} = 1, \dots, a_{\mu}; m = 1, \dots, |\mu| \}$  ( $|\mu|$  is the dimension of  $D^{(\mu)}(\mathbf{G})$ ) of  $\mathcal{S}_D$  is SAB if its vectors satisfy:

$$D(g) | \mu t_{\mu} m \rangle = \sum_{m'=1}^{|\mu|} D_{m'm}^{(\mu)}(g) | \mu t_{\mu} m' \rangle. \quad (1)$$

The direct product of two vectors from different  $\mathbf{G}$ -spaces is a fixed point of  $\mathbf{G}$  iff the transformations of the factors mutually cancel, i.e. iff the factors transform oppositely. This intuitive fact underlies the SAB construction by the modified group projector technique. For each irreducible component  $D^{(\mu)}(\mathbf{G})$  with  $a_{\mu} > 0$ , the initial space  $\mathcal{S}_D$  is directly multiplied by the dual  $\mathcal{H}^{(\mu)*}$  of the space of  $D^{(\mu)}(\mathbf{G})$ . This space carries the auxiliary representation  $\Gamma^{\mu}(\mathbf{G}) \stackrel{\text{def}}{=} D(\mathbf{G}) \otimes D^{(\mu)*}(\mathbf{G})$ ; its fixed point space, i.e. the range  $\mathcal{R}(\mathbf{G}(\Gamma^{\mu}))$  of the modified projector  $\mathbf{G}(\Gamma^{\mu}) \stackrel{\text{def}}{=} \frac{1}{|\mathbf{G}|} \sum_g \Gamma^{\mu}(g)$ , contains exactly all the vectors with  $\mathcal{S}_D$  factors transforming according to  $D^{(\mu)}(\mathbf{G})$ . Any basis  $\{ | \mu t_{\mu} \rangle | \mu = 1, \dots, a_{\mu} \}$  of  $\mathcal{R}(\mathbf{G}(\Gamma^{\mu}))$  yields the  $\mu$ -part of SAB as the partial scalar products with the standard basis  $\{ | \mu^* m \rangle | m = 1, \dots, |\mu| \}$  of  $\mathcal{H}^{(\mu)*}$ :

$$| \mu t_{\mu} m \rangle = \langle \mu^* m | \mu t_{\mu} \rangle \quad t_{\mu} = 1, \dots, a_{\mu}; m = 1, \dots, |\mu|. \quad (2)$$

If the basis is required to be simultaneously symmetry-adapted and eigen basis (SAEB) of the Hamiltonian  $H$  (naturally,  $H$  commutes with  $D(\mathbf{G})$ ), the vectors  $| \mu t_{\mu} \rangle$  should be chosen as the eigen vectors of  $H \otimes I_{\mu}$  (the identity operator is denoted by  $I$ ). The method is especially powerful when  $D(\mathbf{G})$  has inductive structure  $D(\mathbf{G}) = \delta(\mathbf{S} \uparrow \mathbf{G}) \otimes d(\mathbf{G})$ , where  $\delta(\mathbf{S})$  is representation (called interior) of the subgroup  $\mathbf{S}$  and  $d(\mathbf{G})$  any representation (called exterior) of  $\mathbf{G}$ . Eventual weak-direct product structure of  $\mathbf{G}$  enables further simplifications.

In section 2 the SAB construction for multi orbit systems is considered; it is shown how the interrelation of the tight-binding Hamiltonian and the inductive structure of the state space representation of the symmetry group yields an extremely simple way to get the eigen energies together with the corresponding eigen states. The results are applied to the single wall carbon nanotubes (SWCT) [2, 3] and their symmetry groups [4] in the section 3, to accomplish the full symmetry assignation of the electronic bands and get the corresponding Bloch type symmetry-adapted eigen functions.

## 2. Tight binding Hamiltonian in the induced state space

To introduce notation we briefly review the necessary results on the modified group projector technique for induced representations [1]. Let  $\mathbf{S}$  be a subgroup in  $\mathbf{G}$  with the left transversal  $\mathbf{Z} = \{ z_p | p = 0, \dots, |\mathbf{Z}| - 1 \}$  (by convention,  $z_0$  is the identity element  $e$  and  $|\mathbf{Z}| = |\mathbf{G}|/|\mathbf{S}|$ ). Then for any fixed  $g \in \mathbf{G}$  and  $z_p \in \mathbf{Z}$  there are unique  $s(g, z_p) \in \mathbf{S}$  and the index  $p(g)$  satisfying  $g = z_p s(g, z_p) z_{p(g)}^{-1}$  (e.g. for  $g = z_p$ ,  $s(z_p, z_p) = z_{p(z_p)} = e$ , i.e.  $p(z_p) = 0$ ). Given the interior representation  $\delta(\mathbf{S})$  (in the space  $\mathcal{S}_{\delta}$  with the basis  $\{ | \psi \rangle | \psi = 1, \dots, |\delta| \}$ ) and the exterior representation  $d(\mathbf{G})$  (in the



space  $\mathcal{H}_d$ ), we look for SAB of the induced type representation  $D(\mathbf{G}) = \delta(\mathbf{S} \uparrow \mathbf{G}) \otimes d(\mathbf{G})$ . The modified procedure deals with two auxiliary representations for each irreducible component  $D^{(\mu)}(\mathbf{G})$ :  $\Gamma^\mu(\mathbf{G}) = D(\mathbf{G}) \otimes D^{(\mu)*}(\mathbf{G})$  in the space  $\mathcal{S}_{\Gamma^\mu} = \mathcal{S}_D \otimes \mathcal{H}^{(\mu*)} = \oplus_p \mathcal{S}_{p\gamma^\mu}$  (its operators are  $\Gamma^\mu(g) = \sum_p E_{p(g)}^p \otimes \beta_p^\mu \gamma^\mu(s(g, z_p)) \beta_{p(g)}^{\mu\dagger}$ ), and its pulled down subgroup representation  $\gamma^\mu(\mathbf{S}) = \gamma(\mathbf{S}) \otimes D^{(\mu)*}(\mathbf{G} \downarrow \mathbf{S})$  (here  $\gamma(\mathbf{S}) = \delta(\mathbf{S}) \otimes d(\mathbf{G} \downarrow \mathbf{S})$ ; restricted representation denoted by  $\downarrow$ ) in  $\mathcal{S}_{\gamma^\mu} = \mathcal{S}_\delta \otimes \mathcal{H}_d \otimes \mathcal{H}^{(\mu*)}$ . The spaces  $\mathcal{S}_{p\gamma^\mu}$  are the replicas of  $\mathcal{S}_{0\gamma^\mu} = \mathcal{S}_{\gamma^\mu}$ . The matrices  $E_q^p$  (with vanishing all but  $pq$ -th element, which equals 1) are used to switch between these spaces; together with the operators  $\beta_p^\mu = I_\delta \otimes d(z_p) \otimes D^{(\mu)*}(z_p)$  in  $\mathcal{S}_{\gamma^\mu}$  they give the transfer operators  $E_0^p \otimes \beta_p^\mu : \mathcal{S}_{\gamma^\mu} \rightarrow \mathcal{S}_{p\gamma^\mu}$ . The modified group projector  $\mathbf{G}(\Gamma^\mu)$  is essentially equivalent to the pulled down projector  $\mathbf{S}(\gamma^\mu)$  (onto the fixed point space of  $\gamma^\mu(\mathbf{S})$ ) by the partial isometry  $B^\mu : \mathcal{S}_{\gamma^\mu} \rightarrow \mathcal{S}_{\Gamma^\mu}$ :

$$\mathbf{G}(\Gamma^\mu) = B^\mu \{E_0^0 \otimes \mathbf{S}(\gamma^\mu)\} B^{\mu\dagger}, \quad B^\mu = \frac{1}{\sqrt{|Z|}} \sum_t E_0^t \otimes \beta_t^\mu. \quad (3)$$

It has been shown that the basis  $|\mu t_\mu\rangle^0$  of the range of  $\mathbf{S}(\gamma^\mu)$  determines the vectors  $|\mu t_\mu\rangle = B^\mu |\mu t_\mu\rangle^0$ , resulting in the SAB  $|\mu t_\mu m\rangle$  given by (2):

$$|\mu t_\mu m\rangle = \langle \mu^* m | (B^\mu |\mu t_\mu\rangle^0). \quad (4)$$

We generalize these results to the case when  $D(\mathbf{G}) = \oplus_P D^P(\mathbf{G})$  is direct sum of the several induced-type representations from the subgroups  $\mathbf{S}^P$  (with the transversals  $\mathbf{Z}^P$ ) and the interior representations  $\delta^P(\mathbf{S}^i)$ , i.e.  $D^P(\mathbf{G}) = \delta^P(\mathbf{S}^P \uparrow \mathbf{G}) \otimes d(\mathbf{G})$ . It is straightforward to show that the auxiliary representation of the modified technique is already partially reduced in the inductive spaces  $\mathcal{S}_{\Gamma^{P\mu}}$ :  $\Gamma^\mu(\mathbf{G}) = D(\mathbf{G}) \otimes D^{(\mu)*}(\mathbf{G}) = \oplus_P \Gamma^{P\mu}(\mathbf{G})$ , where  $\Gamma^{P\mu}(\mathbf{G}) = D^P(\mathbf{G}) \otimes D^{(\mu)*}(\mathbf{G})$ . Therefore it is pulled down into the space  $\mathcal{S}_{\gamma^\mu} = \oplus_P \mathcal{S}_{\gamma^{P\mu}}$  for each component  $\Gamma^{P\mu}$  independently, and the transfer operator, mapping  $\mathcal{S}_{\gamma^\mu}$  into  $\mathcal{S}_{\Gamma^\mu}$  is obvious generalization of (3):

$$B^\mu = \sum_P B^{P\mu}, \quad B^{P\mu} = \frac{1}{\sqrt{|\mathbf{Z}^P|}} \sum_{p \in \mathbf{Z}^P} E_{P0}^{Pp} \otimes \beta_p^{P\mu}, \quad (5)$$

with  $\beta_p^{P\mu} = I_{\delta^P} \otimes d(z_p^P) \otimes D^{(\mu)*}(z_p^P)$ . Finally, the pulled down projector is found:

$$\mathbf{G}^\downarrow(\Gamma^\mu) = \sum_P B^{P\mu\dagger} \mathbf{G}(\Gamma^{P\mu}) B^{P\mu} = \sum_P E_{P0}^{P0} \otimes \mathbf{S}^P(\gamma^{P\mu}) \quad (6)$$

Note the possibility to obtain the standard basis independently in each subspace  $\mathcal{S}_{D^P}$  using (4).

Further, let the Hamiltonian be given and SAEb is looked for. Preliminary, we show that  $H$  can be always chosen to act trivially in  $\mathcal{H}_d$ . Suppose  $d(\mathbf{G}) = d'(\mathbf{G}) \otimes d_0(\mathbf{G})$ , and  $H$  acts trivially only in  $\mathcal{H}_{d_0}$ . Due to the equivalence of the representations  $(\delta(\mathbf{S}) \uparrow \mathbf{G}) \otimes d'(\mathbf{G})$  and  $(\delta(\mathbf{S}) \otimes d'(\mathbf{G} \downarrow \mathbf{S})) \uparrow \mathbf{G}$  the non-trivial part can be absorbed in the interior representation, using  $\delta(\mathbf{S}) \otimes d'(\mathbf{G} \downarrow \mathbf{S})$  instead of  $\delta(\mathbf{S})$ . Thus, the Hamiltonian has the form  $H = H' \otimes I_d$  providing its triviality in the external space  $\mathcal{H}_d$ .



Then, by the modified prescription the auxiliary operator  $H_\mu = H \otimes I_\mu$  (in  $\mathcal{S}_D \otimes \mathcal{H}^{(\mu)*}$ ) is pulled down to the space  $\mathcal{S}_{\gamma^\mu}$  by  $B^\mu$  giving

$$H_\mu^\downarrow \stackrel{\text{def}}{=} B^{\mu\dagger} H_\mu B^\mu = \sum_{PQ} E_{Q0}^{P0} \otimes \frac{\sum_{pq} \beta_p^{P\mu\dagger} h_{Qq}^{Pp} \beta_q^{Q\mu}}{\sqrt{|\mathbf{Z}^P| |\mathbf{Z}^Q|}}, \quad (7)$$

where

$$h_{Qq}^{Pp} = \left( \sum_{\phi, \psi} h_{Qq\psi}^{Pp\phi} | \phi \rangle \langle \psi | \right) \otimes I_d \otimes I_\mu. \quad (8)$$

are the (rectangular) submatrices in the decomposition  $H_\mu = \sum_{PQ} \sum_{pq} E_{Qq}^{Pp} \otimes h_{Qq}^{Pp}$ . Commutativity of  $H$  with  $D(\mathbf{G})$  interrelates these matrices: for the transversal elements the conditions  $[H, D(z_p^P)] = 0$  give  $h_{Qq}^{Pp} = (\delta^P(s^P(z_q^Q, z_p^P)) \otimes I_d \otimes I_\mu) h_{Q0}^{Pp(z_q^Q)}$ , and (7) becomes

$$H_\mu^\downarrow = \sum_{PQ} E_{Q0}^{P0} \otimes \frac{\sum_{pq} \gamma^{P\mu\dagger}(s^P(z_q^{Q^{-1}}, z_p^P)) \beta_p^{P\mu\dagger} h_{Q0}^{Pp}}{\sqrt{|\mathbf{Z}^P| |\mathbf{Z}^Q|}}. \quad (9)$$

$H_\mu^\downarrow$  commutes with the projector  $\mathbf{G}^\downarrow(\Gamma^\mu)$ , and the vectors  $| \mu t_\mu \rangle^0$  should be chosen as the eigen vectors of  $H_\mu^\downarrow$  from the range of  $\mathbf{S}(\gamma^\mu)$ :  $H_\mu^\downarrow | \mu t_\mu \rangle^0 = \epsilon_{\mu t_\mu} | \mu t_\mu \rangle^0$  and  $\mathbf{G}^\downarrow(\Gamma^\mu) | \mu t_\mu \rangle^0 = | \mu t_\mu \rangle^0$ . Finally, the expansion (4) gives the vectors  $| \mu t_\mu m \rangle$ . It can be proved that the obtained basis is the wanted SAEB of  $H$ , with the same eigen values  $\epsilon_{\mu t_\mu}$ . To differ from the general standard basis, it may turn out that the vectors  $| \mu t_\mu \rangle^0$  are inevitably combinations of the vectors from various  $\mathcal{S}_{\gamma^{P\mu}}$ . Then the SAEB mixes the states of different spaces  $\mathcal{S}_{D^P}$ , too.

Especially, if all the subgroups  $\mathbf{S}^P$  have common transversal  $\mathbf{Z}$ , and  $\mathbf{Z}$  is itself a subgroup of  $\mathbf{G}$  (i.e. when  $\mathbf{G} = \mathbf{ZS}^P$  — the weak direct product), then  $s^P(z_q^{-1}, z_p) = e$  for any  $p$  and  $q$ , simplifying the pulled down Hamiltonian:

$$H_\mu^\downarrow = \sum_{PQ} E_{Q0}^{P0} \otimes \sum_p \beta_p^{\mu\dagger} h_{Q0}^{Pp}. \quad (10)$$

Let the system  $S$  (e.g. molecule, crystal, multi layer, polymer etc.) with the symmetry group  $\mathbf{G}$  consists of  $\mathbf{G}$  orbits  $S^P$  ( $P = 1, 2, \dots$ ). The corresponding stabilizers and transversals are  $\mathbf{S}^P$  and  $\mathbf{Z}^P$ . Obviously, choosing an atom on the orbit for the initial one, the transversal elements  $z_p^P$  biuniquely correspond to the atoms of that orbit. Thus the atoms of the system are enumerated by the pair  $(Pp)$  of the orbit and the transversal element indices. Each orbit defines the representation  $\delta^P(\mathbf{S}^P)$  related to the studied property. For example, when the vibrational modes and the spin-waves are studied, to each atom the polar- and the axial-vector representation are associated.

In the tight-binding approximation each atom of the orbit  $S^P$  contributes to the relevant state space (of valent electrons)  $\mathcal{S}$  by  $\delta^P$  atomic orbitals  $| (Pp)\psi \rangle$  ( $\psi = 1, \dots, \delta^P$ ) spanning the interior space  $\mathcal{S}_{p\delta^P}$ ; the action of the stabilizer element  $s^P$  on  $| (Pp)\psi \rangle$  gives the linear combination of the orbitals from the same atom,  $\sum_{\phi=1}^{\delta^P} \delta_{\phi\psi}^P(s^P) | (Pp)\phi \rangle$ , defining the interior representation  $\delta^P(\mathbf{S}^P)$  (thus  $\delta^P = | \delta^P(\mathbf{S}^P) |$ ). In this problem there is no external representation  $d(\mathbf{G})$ , i.e. in the



previous expressions it should be omitted (substituted by the trivial representation). Finally, the direct sum of the interior spaces gives the total state space  $\mathcal{S} = \mathcal{S}_D$  where the symmetry group acts by the inductive representation  $D(\mathbf{G}) = \oplus_P \delta^P(\mathbf{S}^P \uparrow \mathbf{G})$ .

Within this model, each atom  $(Pp)$  interacts with  $N^P$  neighbors  $(Pp; n)$  ( $n = 1, \dots, N^P$ ) by a coupling coefficients  $V_{\psi\phi}^{Pn}$  between the valent orbitals (the number of the interacting neighbors and the interactions with them is same for all the atoms of the same orbit due to symmetry). So, the Hamiltonian is

$$H = \sum_P \sum_{n=1}^{N^P} \sum_{p=0}^{|\mathbf{Z}^P|-1} \sum_{\psi=1}^{\delta^P} \sum_{\phi=1}^{\delta^{[Pp;n]}} V_{\psi\phi}^{Pn} | (Pp; n)\phi \rangle \langle (Pp)\psi |, \quad (11)$$

where  $[Pp; n]$  is the orbit of the neighbor  $(Pp; n)$ . Therefore, using in (8) the matrix elements  $h_{Q0\psi}^{Pp\phi} = \sum_{n=1}^{N^Q} V_{\phi\psi}^{Qn} \delta_{(Q0;n)}^{(Pp)}$  ( $\delta_j^i$  is the Kronecker delta) determined by (11), the pulled down Hamiltonian becomes

$$H_\mu^\downarrow = \sum_Q \sum_{n=1}^{N^Q} E_{Q0}^{[Q0;n]0} \otimes \left\{ \gamma_{Q(Q0;n)\mu}^{[Q0;n]\mu^\dagger} \left( \sum_{\phi=1}^{\delta^{[Q0;n]}} \sum_{\psi=1}^{\delta^Q} V_{\phi\psi}^{Qn} | \phi \rangle \langle \psi | \otimes I_\mu \right) \right\}, \quad (12)$$

where  $\gamma_{Qp}^{P\mu} = \sum_q \gamma^{P\mu^\dagger}(s^P(z_q^{Q^{-1}}, z_p^P)) / \sqrt{|\mathbf{Z}^Q| |\mathbf{Z}^{[Q0;n]}|}$ . Finally, when there is common transversal being a subgroup in  $\mathbf{G}$ , (10) reduces to the simple sum over neighbors:

$$H_\mu^\downarrow = \sum_Q \sum_{n=1}^{N^Q} E_{Q0}^{[Q0;n]0} \otimes \left\{ \beta_{(Q0;n)}^{[Q0;n]\mu^\dagger} \left( \sum_{\phi=1}^{\delta^{[Q0;n]}} \sum_{\psi=1}^{\delta^Q} V_{\phi\psi}^{Qn} | \phi \rangle \langle \psi | \otimes I_\mu \right) \right\}. \quad (13)$$

### 3. Single-wall carbon nanotube bands

Symmetry groups  $\mathbf{L}_C$  of chiral  $(n_1, n_2)$ , and  $\mathbf{L}_{ZA}$  of zig-zag  $(n, 0)$  and armchair  $(n, n)$  SWCT ( $C$ ,  $Z$  and  $A$  tubes for short) are the line groups [4] given in the factorized and international notation

$$\mathbf{L}_C = \mathbf{T}_q^r \mathbf{D}_n = \mathbf{L}q_p 22, \quad \mathbf{L}_{ZA} = \mathbf{T}_{2n}^1 \mathbf{D}_{nh} = \mathbf{L}2n_n / mcm, \quad (14)$$

with the translational period  $a = a_0 \sqrt{3q/2n\mathcal{R}}$ . Here  $a_0 = 2.461 \text{\AA}$  is the honeycomb lattice period, while  $n, q, p, r$  and  $\mathcal{R}$  are defined in terms of  $n_1$  and  $n_2$ . The parameters  $\tilde{q}$  and  $q$  are even since  $\tilde{q} = q/n = 2 \pmod{12}$ , while  $n$  and  $p$  are even iff both  $n_1$  and  $n_2$  are even; also  $q > 10$  for the realistic tubes (having diameters  $D = a_0 \sqrt{\mathcal{R}nq/2}/\pi$  greater than  $3.4 \text{\AA}$ ).

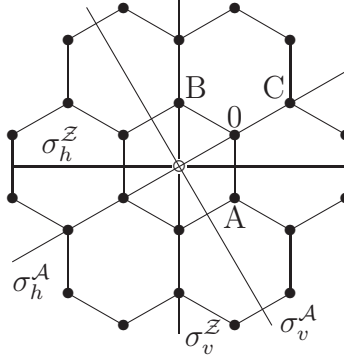
From the factorized notation it follows that these groups are weak-direct products of the cyclic groups generated by  $(C_q^r | a/\tilde{q})$ ,  $C_n$  and  $U$  for  $\mathbf{L}_C$ , and additionally  $\sigma_x$  for  $\mathbf{L}_{ZA}$  (see figure 1). Thus, their elements are monomials

$$\ell(t, s, u, v) = (C_q^r | \frac{a}{\tilde{q}})^t C_n^s U^u \sigma_x^v \quad (15)$$

for  $t = 0, \pm 1, \dots$ ,  $s = 0, \dots, n-1$ ,  $u = 0, 1$ , and  $v = 0$  in  $\mathbf{L}_C$  and  $v = 0, 1$  in  $\mathbf{L}_{ZA}$ .

Each SWCT is a single orbit of its line group. The type of the orbit according to the classification of [5], its stabilizer and the transversal are given in the table 1. In all





**Figure 1.** Nearest neighbors of the C-atom atom denoted by 0, are the atoms 1, 2 and 3. Perpendicular to the figure at  $\circ$  is  $U$ -axis being also  $x$ -axis of the coordinate system;  $\sigma_{h/v}^{Z/A}$  stands for vertical and horizontal mirror planes of  $\mathcal{Z}$  and  $\mathcal{A}$  tubes.

**Table 1.** Orbits and neighbors of SWCT. For  $\mathcal{C}$ ,  $\mathcal{Z}$  and  $\mathcal{A}$  tubes their line group, orbit type, stabilizer and transversal group are in the columns  $\mathbf{G}$ ,  $\mathbf{O}$ ,  $\mathbf{S}$  and  $\mathbf{Z}$ . Then follow the parameters  $t_n$  and  $s_n$  ( $u_n = 1$ ) expressing the three nearest neighbors of the initial atom in the form  $(000; n) = C_{t_n s_n 1}$ .

	$\mathbf{G}$	$\mathbf{O}$	$\mathbf{S}$	$\mathbf{Z}$	$(000; 1)$	$(000; 2)$	$(000; 3)$
$\mathcal{C}$	$\mathbf{L}_{\mathcal{C}}$	$a_1$	$\{e\}$	$\mathbf{T}_q^r \mathbf{D}_n$	$t_1 = -\frac{n_2}{n}$ $s_1 = \frac{2n_1 + (1+r\mathcal{R})n_2}{q\mathcal{R}}$	$t_2 = \frac{n_1}{n}$ $s_2 = \frac{(1-r\mathcal{R})n_1 + 2n_2}{q\mathcal{R}}$	$t_3 = t_1 + t_2$ $s_3 = s_1 + s_2$
$\mathcal{Z}$	$\mathbf{L}_{\mathcal{Z}\mathcal{A}}$	$b_1$	$\{e, C_n \sigma_x\}$	$\mathbf{T}_{2n}^1 \mathbf{D}_n$	$t_1 = 0 \quad s_1 = 1$	$t_2 = 1 \quad s_2 = 0$	$t_3 = 1 \quad s_3 = 1$
$\mathcal{A}$	$\mathbf{L}_{\mathcal{Z}\mathcal{A}}$	$d_1$	$\{e, \sigma_h\}$	$\mathbf{T}_{2n}^1 \mathbf{D}_n$	$t_1 = -1 \quad s_1 = 1$	$t_2 = 1 \quad s_2 = 0$	$t_3 = 0 \quad s_3 = 1$

the cases the transversal is the group  $\mathbf{T}_q^r \mathbf{D}_n$  used to enumerate the atoms: initial atom  $C_{000}$  has the radius vector in the cylindrical coordinate system of figure 1:

$$\mathbf{r}_{000} = \left(\frac{D}{2}, \phi_0, z_0\right), \quad \phi_0 = 2\pi \frac{n_1 + n_2}{nq\mathcal{R}}, \quad z_0 = \frac{n_1 - n_2}{\sqrt{6nq\mathcal{R}}} a_0. \quad (16)$$

The transversal element  $\ell(t, s, u, 0)$  maps  $C_{000}$  to the atom  $C_{tsu}$  with the coordinates  $\mathbf{r}_{tsu} = (D/2, (-1)^u \phi_0 + 2\pi(t/q + s/n), (-1)^u z_0 + tna/q)$ . Experimental data verified the validity of the simple tight-binding nearest neighbors model. Each C atom contributes by one  $p^\perp$  (i.e. graphene  $p_z$ ) orbital  $|tsu\rangle$  (the notation is simplified: the capital and the Greek indices for orbits and interior space vectors, taking on only the value 1, are omitted). The orbital  $|tsu\rangle$  spans the (one dimensional) interior space carrying the trivial stabilizer representation  $\delta(\mathbf{S}) = 1(\mathbf{S})$  (triviality is obvious for  $\mathcal{C}$  tubes, and for the  $\mathcal{Z}$  and  $\mathcal{A}$  ones it follows from the polar-vector type of the  $Y_{l=1}^m$  spherical harmonics involved in  $p^\perp$  orbital). Thus in the total independent electron space  $\mathcal{S}$ , being spanned by all these orbitals, the symmetry group acts by the induced representation  $D(\mathbf{G}) = 1(\mathbf{S} \uparrow \mathbf{G})$ . The pulled down modified projector with the irreducible representation  $D^{(\mu)}(\mathbf{G})$  (see appendix) becomes  $\mathbf{S}(D^{(\mu)*}) = \sum_{s \in \mathbf{S}} D^{(\mu)*}(s) / |\mathbf{S}|$ , and the dimension of its range gives the frequency number of  $D^{(\mu)}(\mathbf{G})$  in  $D(\mathbf{G})$ . The Hamiltonian confines the interaction to the 3 nearest neighbors (see figure 1). Therefore, the pulled down



**Table 2.** Bands and symmetry-adapted eigen vectors of the carbon nanotubes. For each irreducible component  $D^{(\mu)}(\mathbf{L})$  of  $D(\mathbf{L}) = 1(\mathbf{S} \uparrow \mathbf{L})$  its frequency number  $a_\mu$ , energies  $\epsilon_{\mu t_\mu}$ , the transfer operator  $\beta_{tsu}^\mu$  and the pulled down standard eigen basis  $|\mu t_\mu\rangle^0$  are given. For the matrices  $M_2, K_2, O_2, M_4, K_4$  and  $O_4$  see the appendix.

$\mathcal{C}$	$a_\mu$	$\epsilon_{\mu t_\mu}/V$	$\beta_{tsu}^\mu$	$ \mu t_\mu\rangle^0$
$0A_m^\Pi$	1	$\Pi(1 + 2e^{i\frac{m\pi}{q}})$	$\Pi^u e^{im(rt+s\bar{q})\frac{2\pi}{q}}$	$ 0m\Pi\rangle$
$\pi A_m^\Pi$	1	$-\Pi$	$\Pi^u e^{i(m(rt+s\bar{q})\frac{2\pi}{q} + \frac{t\pi}{q})}$	$ \pi m\Pi\rangle$
$kE_m$	2	(18a)	$K_2(\frac{kt}{\bar{q}})M_2(m\frac{tr+s\bar{q}}{\bar{q}})O_2^u$	$ km\rangle,   -k, -m\rangle$
$0\tilde{A}_{\tilde{m}}^\Pi$	1	$\Pi(1 + 2e^{i\frac{m\pi}{n}})$	$\Pi^u e^{i\tilde{m}s\frac{2\pi}{n}}$	$ 0\tilde{m}\Pi\rangle$
$\tilde{\pi}A_{\tilde{m}}^\Pi$	1	$-\Pi$	$\Pi^u (-1)^t e^{i\tilde{m}s\frac{2\pi}{n}}$	$ \tilde{\pi}\tilde{m}\Pi\rangle$
$\tilde{k}E_{\tilde{m}}$	2	(18a)	$K_2(\frac{\tilde{k}}{\bar{q}})M_2(s\tilde{m})O_2^u$	$ \tilde{k}m\rangle,   -\tilde{k}, -\tilde{m}\rangle$
$\mathcal{Z}$	$a_\mu$	$\epsilon_{\mu t_\mu}/V$	$\beta_{tsu}^\mu$	$ \mu t_\mu\rangle^0$
$0A_m^\Pi$	1	$\Pi(1 + 2e^{i\frac{m\pi}{n}})$	$\Pi^u e^{i\frac{m\pi}{n}t}$	$ 0m\Pi A\rangle$
$0E_m^\Pi$	1	$\Pi(1 + 2\cos\frac{m\pi}{n})$	$\Pi^u M_2(-\frac{2s+t}{2}m)O_2^u$	$\frac{ 0m\Pi\rangle + e^{i\frac{m2\pi}{n}} 0, -m, \Pi\rangle}{\sqrt{2}}$
$kE_m^A$	2	$\pm\sqrt{5 + 4e^{i\frac{m\pi}{n}}\cos\frac{ka}{2}}$	$e^{i\frac{m\pi}{n}t}K_2(\frac{kt}{2})O_2^u$	$ kmA\rangle,   -k, m, A\rangle$
$\pi E_{\frac{n}{2}}^\Pi$	1	$-\Pi$	$i^t(-1)^s \Pi^u K_2(\frac{t\pi}{2a})$	$\frac{ \frac{\pi}{a}, \frac{n}{2}, \Pi\rangle -  \frac{\pi}{a}, -\frac{n}{2}, \Pi\rangle}{\sqrt{2}}$
$kG_m$	2	(18b)	$K_4(\frac{kt}{2}, m\frac{t+2s}{2})O_4^u$	$\frac{ km\rangle + e^{-i\frac{m2\pi}{n}} k, -m\rangle}{\sqrt{2}}$ $\frac{ -k, m\rangle + e^{-i\frac{m2\pi}{n}} -k, -m\rangle}{\sqrt{2}}$
$\mathcal{A}$	$a_\mu$	$\epsilon_{\mu t_\mu}/V$	$\beta_{tsu}^\mu$	$ \mu t_\mu\rangle^0$
$0\Pi_m^+$	1	$1 + 2e^{i\frac{m\pi}{n}}$	$\Pi^u e^{i\frac{m\pi}{n}t}$	$ 0, m, +, \Pi\rangle$
$0E_m^+$	2	$\pm\sqrt{5 + 4\cos\frac{m\pi}{n}}$	$\Pi^u M_2(-\frac{2s+t}{2}m)O_2^u$	$ 0m+\rangle,  0, -m, +\rangle$
$kE_m^\Pi$	1	$\Pi(1 + 2e^{i\frac{m\pi}{n}}\cos\frac{ka}{2})$	$\Pi^u e^{i\frac{m\pi}{n}t}K_2(\frac{kt}{2})O_2^u$	$\frac{ km\Pi\rangle +  -k, m, \Pi\rangle}{\sqrt{2}}$
$\pi E_{\frac{n}{2}}^\Pi$	1	$-3\Pi$	$i^t(-1)^s (\pm 1)^u K_2(\frac{t\pi}{2a})$	$\frac{ \frac{\pi}{a}, \frac{n}{2}, \Pi\rangle + \Pi \frac{\pi}{a}, -\frac{n}{2}, \Pi\rangle}{\sqrt{2}}$
$kG_m$	2	(18c)	$K_4(\frac{kt}{2}, m\frac{t+2s}{2})O_4^u$	$\frac{ km\rangle +  k, -m\rangle}{\sqrt{2}}$ $\frac{ -k, m\rangle +  -k, -m\rangle}{\sqrt{2}}$

Hamiltonian reads:

$$H_\mu^\dagger = \sum_{n=0}^3 V_n D^{(\mu)*\dagger}(\ell(t_n, s_n, u_n, 0)). \quad (17)$$

Here,  $\ell(t_n, s_n, u_n, 0)$  is the transversal element which maps the initial atom into its neighbor  $(000; n)$ ; it is given in table 1. By  $n = 0$  the initial atom itself is included (the diagonal term of the Hamiltonian); nevertheless, its contribution to the energy is reduced to the additive constant  $V_0$ , and hereafter it is omitted. Further, since the rolling up induced distortions of the honeycomb lattice are nearly homogeneous, all the remaining coupling constants are approximately equal:  $V_1 = V_2 = V_3 = V$  (estimated between  $-2.7\text{eV}$  and  $-2.5\text{eV}$ ).

Finally, using the irreducible representations from the appendix and the data from table 1, the Hamiltonian and the modified projectors are pulled down and the results are given in table 2. The most general dispersion relations for the bands of  $\mathcal{C}$ ,  $\mathcal{Z}$  and  $\mathcal{A}$



tubes are respectively:

$$\epsilon_{E_m}^{\pm}(k) = \pm V \sqrt{1 + 8 \cos \frac{\psi_A}{2} \cos \frac{\psi_B}{2} \cos \frac{\psi_A - \psi_B}{2}}, \quad (18a)$$

$$\epsilon_{G_m}^{\pm}(k) = \pm V \sqrt{1 + 4 \cos \frac{ka}{2} \cos \frac{m\pi}{n} + 4 \cos^2 \frac{m\pi}{n}}, \quad (18b)$$

$$\epsilon_{G_m}^{\pm}(k) = \pm V \sqrt{1 + 4 \cos \frac{ka}{2} \cos \frac{m\pi}{n} + 4 \cos^2 \frac{ka}{2}}. \quad (18c)$$

The angles used in (18a) are

$$\psi_A = -ka \frac{n_2}{q} + 2\pi m \frac{2n_1 + n_2}{qn\mathcal{R}}, \quad \psi_B = ka \frac{n_1}{q} + 2\pi m \frac{n_1 + 2n_2}{qn\mathcal{R}}. \quad (19)$$

Substituting them in (18a) by

$$\tilde{\psi}_A = -\tilde{k}a \frac{n_2}{q} + 2\pi \tilde{m} \frac{2n_1 + (1 + r\mathcal{R})n_2}{qn\mathcal{R}}, \quad \tilde{\psi}_B = \tilde{k}a \frac{n_1}{q} + 2\pi \tilde{m} \frac{(1 - r\mathcal{R})n_1 + 2n_2}{qn\mathcal{R}}, \quad (20)$$

the  $\tilde{k}\tilde{m}$  bands are obtained. To find the standard basis  $|\mu t_\mu m\rangle$  it suffices to apply (4), with  $\beta_{tsu}^\mu$  and  $|\mu t_\mu\rangle^0$  given in table 2. For example, the bands of the representations  ${}_k E_m^{\Pi^v}$  of the  $\mathcal{Z}$  and  $\mathcal{A}$  tubes corresponds to the symmetry adapted generalized Bloch states:

$$|km\Pi^v\rangle = \sum_{ts} e^{i(m\frac{\pi}{n} + k\frac{a}{2})t} |(ts0)\rangle, \quad |-k, m, \Pi^v\rangle = \Pi^v \sum_{ts} e^{i(m\frac{\pi}{n} - k\frac{a}{2})t} |(ts1)\rangle. \quad (21)$$

#### 4. Summary

The modified group projector technique is applied to find the symmetry adapted basis for the sum  $D(\mathbf{G}) = \oplus_P \delta^P(\mathbf{S}^P \uparrow \mathbf{G}) \otimes d(\mathbf{G})$  of the induced interior representations  $\delta^P(\mathbf{S}^P)$  of arbitrary subgroups  $\mathbf{S}^P$  of  $\mathbf{G}$  directly multiplied by the exterior representation  $d(\mathbf{G})$ . It is shown that this basis is expanded basis  $|\mu t_\mu\rangle^0$  of the range of the pulled down projector  $\mathbf{G}^\downarrow(\Gamma^\mu) = \sum_P E_{P0}^{P0} \gamma^{P\mu}(\mathbf{S}^P)$  in the low dimensional auxiliary space (summed interior spaces multiplied by the exterior and dual irreducible space). The same procedure is applied when the standard basis, being also the eigen basis of the Hamiltonian  $H$  (acting trivially in the exterior space) is looked for: then in the range of  $\mathbf{G}^\downarrow(\Gamma^\mu)$  the eigen vectors  $|\mu t_\mu\rangle^0$  of the pulled down Hamiltonian  $H_\mu^\downarrow$  are to be found. In particular, for the general tight-binding Hamiltonian the operators  $H_\mu^\downarrow$  are found.

It is interesting to understand the physical meaning of the operator  $\gamma_{Qp}^{P\mu}$  appearing in (12). In fact, the different transversals  $\mathbf{Z}^P$  and  $\mathbf{Z}^Q$  arrange the atoms on the corresponding orbits differently. Even when the two orbits have the same transversal, since in general it is not a subgroup, the successive elements are not arranged homogeneously. Thus, the sum over the orbit  $S^Q$  involved in  $\gamma_{Qp}^{P\mu}$  gives the average relative positions between  $S^Q$  and  $S^P$ . The terms in the sum are mutually equal when the relative positions of the atoms on the two orbits are constant, provided by the homogeneous action of the same transversal when it is a subgroup.



**Table A1.** Irreducible representations of  $\mathbf{L}_C$  classified by the  $km$  and  $\tilde{k}\tilde{m}$  quantum numbers. For the irreducible representations denoted in the first column, possible values of  $k$  and  $m$  ( $\tilde{k}$  and  $\tilde{m}$ ) are given in the second column, and then the matrices of the generators follow. Finally, SAB is given in terms of quantum numbers. Only for integer  $m = n/2, q/2, -p/2, (q-p)/2$  the corresponding representations appear. (\*)  $k = 0$  with  $m \in (0, \frac{q}{2})$ , and  $k = \frac{\pi}{a}$  with  $m \in (-\frac{p}{2}, \frac{q-p}{2})$  and  $k \in (0, \frac{\pi}{a})$  with  $m \in (-\frac{q}{2}, \frac{q}{2}]$ .

IR	$(k, m)$	$(C_q^r   \frac{a}{q})$	$C_n$	$U$	SAB
${}_k A_m^{\Pi^U}$	$k=0, m=0, \frac{q}{2}$ $k=\frac{\pi}{a}, m=-\frac{p}{2}, \frac{q-p}{2}$	$e^{i(mr\frac{2\pi}{q} + k\frac{a}{q})}$	$e^{im\frac{2\pi}{n}}$	$\Pi^U$	$  km \Pi^U \rangle$
${}_k E_m$	(*)	$M_2(\frac{mr}{q}) K_2(\frac{k}{q})$	$M_2(m)$	$O_2$	$\begin{matrix}   km \rangle \\   -k, -m \rangle \end{matrix}$
$_{\tilde{k}} A_{\tilde{m}}^{\Pi^U}$	$\tilde{k} = 0, \tilde{q}\frac{\pi}{a}, m = 0, \frac{n}{2}$	$e^{i\tilde{k}\frac{a}{q}}$	$e^{i\tilde{m}\frac{2\pi}{n}}$	$\Pi^U$	$  \tilde{k}\tilde{m} \Pi^U \rangle$
$_{\tilde{k}} E_{\tilde{m}}$	$k=0, \tilde{q}\frac{\pi}{a}, m \in (0, \frac{n}{2})$ $k \in (0, \tilde{q}\frac{\pi}{a}), m \in (-\frac{n}{2}, \frac{n}{2}]$	$K_2(\frac{\tilde{k}}{q})$	$M_2(\tilde{m})$	$O_2$	$\begin{matrix}   \tilde{k}\tilde{m} \rangle \\   -\tilde{k}, -\tilde{m} \rangle \end{matrix}$

These results enable simple calculation of the crystal energy bands, with automatic assignation of the bands by the symmetry quantum numbers. The method is applied to find the energy bands and corresponding eigen functions of the carbon nanotubes [2]. Although the bands dispersion relations have been already calculated in the literature both for  $km$  [3, 6], and  $\tilde{k}\tilde{m}$  quantum numbers [7, 8, 9, 10], only the helical part of the symmetry group has been used, neglecting the parities. Such incomplete band assignation can produce errors in studying various processes, since the selection rules incorporating parities are more severe, forbidding some otherwise allowed interband transitions. Also the generalized Bloch eigen functions have the most precise form only when the full symmetry is used. The necessity for full symmetry group treatment is enforced by the fact that the peaks of the density of states mostly correspond to the even or odd states, i.e. to the representations with parities. This and some other symmetry related questions (e.g. topology of bands, including band sticking and metallic properties) will be analyzed elsewhere.

## Appendix A. Irreducible representations of $\mathbf{L}_C$ and $\mathbf{L}_{\mathcal{Z}\mathcal{A}}$

There are two physically based classification of the irreducible representations of the nonsymmorphic line groups (like the considered ones), differing in used quasi momenta: quantum numbers labeling representations may be either  $k$  and  $m$  of linear and angular quasi momenta, or  $\tilde{k}$  and  $\tilde{m}$  of helical (includes linear and a part of angular) and remaining angular momemnta. As for the  $\mathcal{C}$  tubes both are used in literature (see e.g. [3, 6] for  $km$  and [7, 8, 9, 10] for  $\tilde{k}\tilde{m}$  classification), while for the  $\mathcal{Z}$  and  $\mathcal{A}$  tubes only the former one, as it has been done in this paper.

Due to  $U$  axis in  $\mathbf{L}_C$  and  $\mathbf{L}_{\mathcal{Z}\mathcal{A}}$  the linear quasi momentum  $k$  runs over the irreducible domain  $[0, \pi/a]$  (and  $\tilde{k} \in [0, \tilde{\pi}]$  with  $\tilde{\pi} = \tilde{q}\pi/a$ ) being the half of Brillouine zone. In its interior the representations are grouped in the  $k$ -series differing by  $m$  (or  $\tilde{k}$ -series differing by  $\tilde{m}$ ). At the boundaries some representations of  $\mathbf{L}_C$  have  $U$ -parity quantum number



**Table A2.** Irreducible representations of  $\mathbf{L}_{\mathcal{ZA}}$  classified by the  $km$  quantum numbers. For the irreducible representations denoted in the first column allowed values of  $k$  and  $m$  are given in the second column, and then the matrices of the generators follow. Finally, SAB is given in terms of quantum numbers. Only for  $n$  even  $\pi E_{n/2}^{\Pi^U}$  appears. The four dimensional matrices are  $M_4(m) = I_2 \otimes M_2(m)$ ,  $K_4(k, m) = K_2(k) \otimes M_2(m)$  and  $V_4 = I_2 \otimes O_2$ .

IR	$(k, m)$	$(C_{2n}^1   \frac{a}{2})$	$C_n$	$U$	$\sigma_x$	SAB
${}_0A/B_m^{\Pi^h}$	$k = 0, m = 0, n$	$e^{im\frac{\pi}{n}}$	1	$\Pi^h \Pi^v$	$\Pi^v$	$ 0m\Pi^h\Pi^v\rangle$
${}_0E_m^{\Pi^h}$	$k = 0, m \in (0, n)$	$M_2(\frac{m}{2})$	$M_2(m)$	$\Pi^h O_2$	$O_2$	$ 0m\Pi^h\rangle$ $ 0, -m, \Pi^h\rangle$
${}_kE_m^{A/B}$	$k \in (0, \frac{\pi}{a}), m = 0, n$ $k = \frac{\pi}{a}, m = 0$	$e^{i\frac{m\pi}{n}} K_2(\frac{k}{2})$	$I_2$	$\Pi^v O_2$	$\Pi^v I_2$	$ km\Pi^v\rangle$ $ -k, m, \Pi^v\rangle$
$\pi E_{\frac{n}{2}}^{\Pi^U}$	$k = \frac{\pi}{a}, m = \frac{n}{2}$	$iK_2(\frac{\pi}{2a})$	$-I_2$	$\Pi^U I_2$	$O_2$	$ \frac{\pi}{a}, \frac{n}{2}, \Pi^U\rangle$ $ \frac{\pi}{a}, -\frac{n}{2}, \Pi^U\rangle$
${}_kG_m$	$k \in (0, \frac{\pi}{a}), m \in (0, n)$ $k = \frac{\pi}{a}, m \in (0, \frac{n}{2})$	$K_4(\frac{k}{2}, \frac{m}{2})$	$M_4(m)$	$O_4$	$V_4$	$ km\rangle,  k, -m\rangle,$ $ -k, m\rangle,  -k, -m\rangle$

$\Pi^U = \pm 1$  denoted as the superscript  $+/-$ . As for the group  $\mathbf{L}_{\mathcal{ZA}}$  the superscript  $+/-$  stands for  $\sigma_h$ -parity (with respect to the horizontal mirror plane  $\sigma_h = U\sigma_x$ )  $\Pi^h = \pm 1$ , except for the representations  $\pi E_{n/2}^{\pm}$  where it corresponds to  $\Pi^U = \pm 1$ ; additionally, some of the  $k$ -series and boundary representations of  $\mathbf{L}_{\mathcal{ZA}}$  have quantum number of  $\sigma_x$ -parity  $\Pi^v = \pm 1$ , denoted by  $A/B$ , respectively. The representations are given by the matrices of the group generators. In the tables  $I_n$  and  $O_n$  stand for  $n$ -dimensional diagonal and off-diagonal unit matrices respectively, while the two dimensional diagonal matrices are  $M_2(m) = \text{diag}[e^{im2\pi/n}, e^{-im2\pi/n}]$ ,  $K_2(k) = \text{diag}[e^{ika}, e^{-ika}]$ .

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